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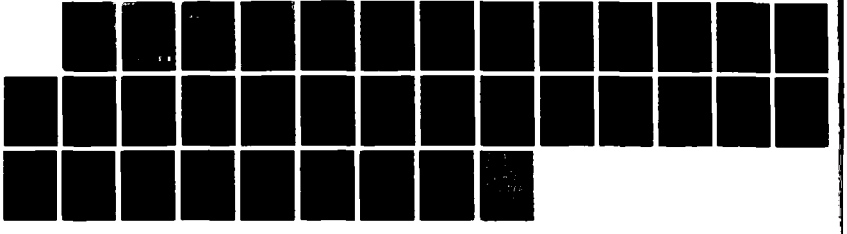

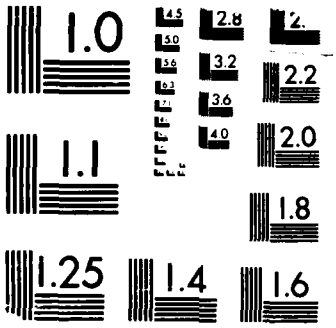

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AFGL-TR-88-0026

PROGRESS ON A MONTE CARLO SHUTTLE CONTAMINATION MODEL.

James B. Elgin

Spectral Sciences, Inc.
111 South Bedford Street
Burlington, MA 01803

1 February 1988

Scientific Report No. 2

AIR FORCE GEOPHYSICS LABORATORY
AIR FORCE SYSTEMS COMMAND
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Progress is described in the development of the SOCRATES model of the space shuttle orbiter contamination. New code features, including surface flux statistics and a plume core model are discussed, and a sample problem is shown for the contamination from an RCS engine operating at 200 km altitude.

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CONTENTS

ILLUSTRATIONS

1. INTRODUCTION

This is the second yearly scientific report on a three year effort to develop a Monte Carlo model of contamination for the space shuttle orbiter. Contamination of instruments on the space shuttle orbiter is an issue of major concern. The shuttle gives off matter through surface outgassing, via various thrusters and from flash evaporators. At altitudes where the atmospheric mean free path is comparable to or less than shuttle dimensions, the deposition back onto shuttle-borne instruments will be largely determined by the multiple collision environment surrounding the shuttle. Even at higher altitudes, this may be the dominant source of contaminants for some portions of the shuttle. In addition to physical contamination of shuttle surfaces, "radiation contamination" is also a potential problem as gases surrounding the shuttle collide at high speed with atmospheric molecules. These energetic collisions can lead to vibrational excitation and subsequent radiative decay. A similar issue of some concern is the presence of ions in the vicinity of the shuttle which can (possibly) be produced via the critical ionization velocity effect. Ions in the shuttle environment may remain there for some time due to electric field forces, and radiative recombination is another potential source of radiation contamination. The situation is depicted schematically in Figure 1.

Spectral Sciences, Inc., (SSI) is developing a three dimensional Monte Carlo model of the flow field about the shuttle so that the contamination can be accurately characterized and understood. A comprehensive model of the contaminant field surrounding the space shuttle orbiter is crucial to the design of experiments which are to fly on the shuttle and to the development of procedures for minimizing the contamination.

SSI is adapting an existing three dimensional plume code (CHIMERA) to the space shuttle problem. The code is designed in a highly modularized fashion, so that additional physical and geometric complexity can be added as deemed necessary without requiring major rewriting of the model. The existing code already treats complex chemical and photochemical reactions for a neutral gas composed of molecules with energy dependent collision cross sections. The model allows for internal degrees of freedom for the molecules which can exchange energy with the translational mode. It has been named the SOCRATES code, which is an acronym for Shuttle Orbiter Contamination Representation Accounting for Transiently Emitted Species.

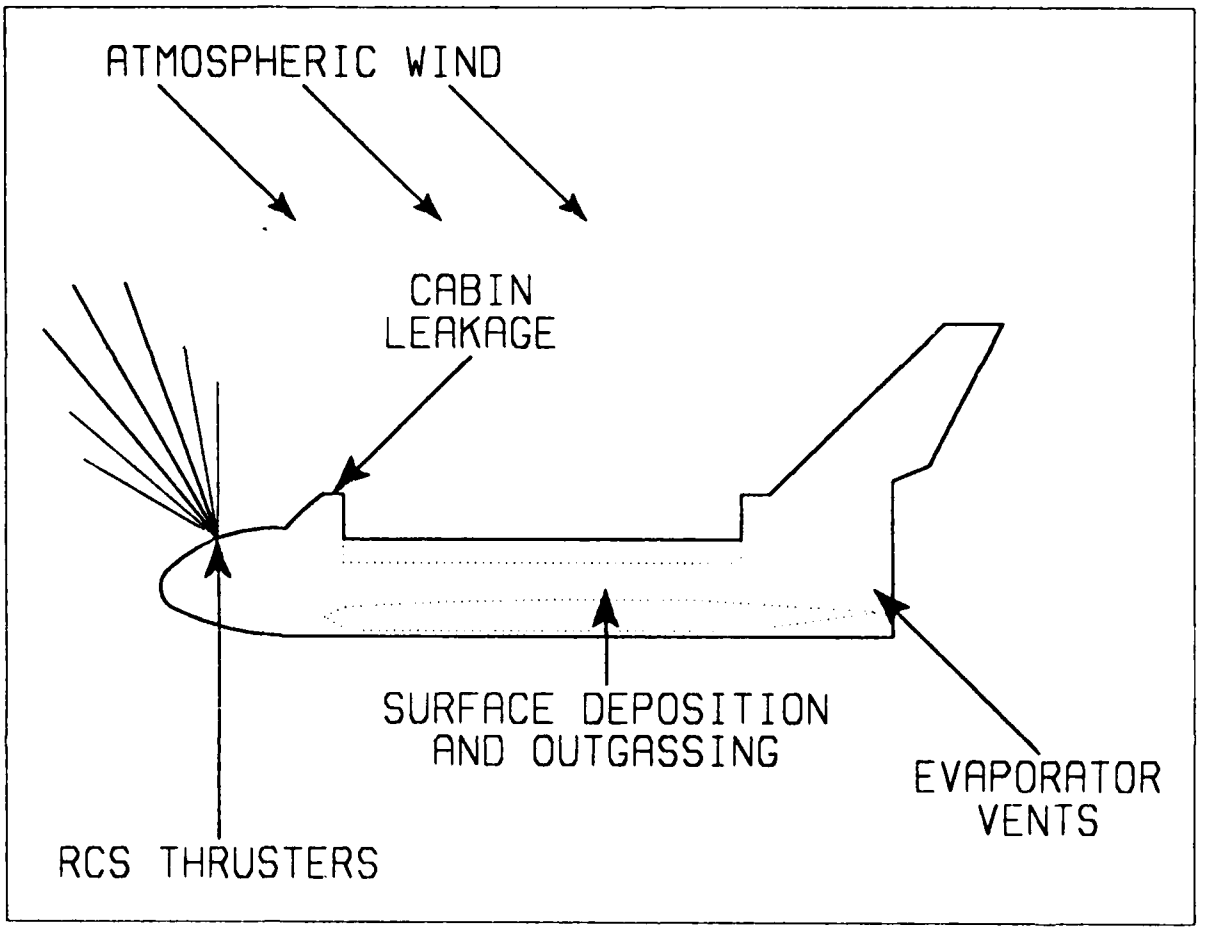

Figure 1. A Schematic Representation of the Major Elements of the Shuttle Contamination Problem.

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2. SUMMARY OF WORK PERFORMED IN THE FIRST YEAR

The first year's work was discussed in detail in the previous yearly report[1]; it is merely summarized here to provide a frame of reference for the work performed in the second year.

2.1 Shuttle Representation

A preliminary version of the shuttle was constructed. This model was intentionally simplified since it made no sense to deal in precise geometric detail before the code was checked out. The initial model for the shuttle geometry was designed to form a completely closed (i.e., no "holes"), non-overlapping surface which approximated the shuttle geometry with a minimum number of surface elements. The surface elements were simple geometric shapes such as rectangles, triangles, disks, cylinders and cones. This first model employed four surface types with a total of eleven surface elements. For production runs, this simplified representation will be replaced by available more accurate representations.

2.2 Determination of Surface Intersections

The calculation of an intersection point between a molecular trajectory and the shuttle, while conceptually straightforward, is a potential source of considerable computational effort. Routines were written to calculate the intersection point in space and time for a molecule starting from an arbitrary position and velocity for each of the simple geometric shapes (triangles, rectangles, etc.) used in the shuttle description. These routines also return the local triple of unit vectors at the intersection point which is needed for the calculation of surface reflections.

Given the routines to provide intersections with the basic surface elements, it was still not trivial to implement them into the Monte Carlo simulation in an efficient fashion. There are thousands of molecules (sometimes over a hundred thousand) in a simulation, and each one of these molecules is advanced along its trajectory at every solution time step. Some check for intersection must be made for each molecule, at every time step, for every surface element of which the shuttle model is comprised. (It is not valid to stop checking for intersections when one is found for, say, surface element "A", since there may be another surface element, "B", shielding "A". It is the first intersection point along the molecular trajectory which is the relevant one.) Hence, it was desirable to have an algorithm which performed this computation as efficiently as possible.

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1. Elgin, J. B., and Sundberg, R. L., "Development of a Monte Carlo Shuttle Contamination Model," Spectral Sciences, Inc. Rpt. No. SSI-TR-113, September 1986. Prepared for Air Force Geophysics Laboratory, Hanscom AFB, MA, under Rpt. No. AFGL-TR-86-0204. AD175409

A concept to speed up the calculation of surface intersections was implemented. An element was added to the "state vector" to indicate the time at which a given molecule will experience a surface collision if its trajectory is not altered. (The state vector is simply the entire list of information which the code has about each simulated molecule.) The element is used as follows:

1) Whenever a molecule is introduced into the simulation, this element is set to zero. This serves as a flag indicating that a possible surface intersection has not yet been calculated for this molecule.

2) During collision sampling, whenever a molecule has its trajectory changed, the state vector element for surface intersection is reset to zero. This flags the molecule to have its possible surface intersection recomputed when it is advanced along its trajectory.

3) The routines which advance a molecule along its trajectory examine this element. If it is zero, then all surfaces are checked for possible intersection. If an intersection is found, then the time at which the intersection will take place is put in the state vector element. If it is determined that the current trajectory will not intersect any surfaces, then the value of 10^{20} (a computer approximation for infinity) is put in the element.

4) If it is known that a molecule will not intersect a surface within the time interval corresponding to the molecular advancement, then the molecule is simply moved along its trajectory without further checking of surfaces. This is the case for the large majority of molecules which are inspected.

5) If a molecule does intersect a surface within the current time interval, then it is advanced to the point of intersection. The state vector corresponding to the post-reflection conditions are calculated and the element corresponding to surface collision time is reset to zero. The molecule is then advanced along its new trajectory for the remainder of the time interval, allowing for any new reflections which may occur.

2.3 Surface Reflections

Routines were written to describe a diffuse reflection of a molecule from a surface after complete accommodation. This is felt to be the most

reasonable physical model, so it is the natural initial choice. Other options (in particular sticking) will be added as the model is expanded.

2.4 Grid Structure Changes

The cell geometry for the CHIMERA plume code was based on cylindrical polar coordinates so it could naturally yield the axisymmetric limit for a plume aligned with the free stream. Additionally, it utilized the symmetry plane that exists when an initially axisymmetric plume interacts with a uniform atmosphere. This enabled half of the overall solution to be inferred from the other half.

The symmetry plane does not exist for the shuttle problem and cannot be used. Similarly, there is no reason to utilize the cylindrical polar coordinate system for the cell geometry since the axisymmetric limit does not exist. Hence, the grid structure was changed to a more convenient three dimensional Cartesian coordinate system. There are parameters for varying the number and spacings of the cells independently in all six directions from the origin, so cells will not be placed where they are not needed.

The alteration of the cell grid structure required the following changes to the code:

1) The initialization routines calculating cell volumes and boundary locations had to be modified.

2) The procedure to determine the cell in which a molecule resides from its position had to be altered.

3) The routines to introduce new atmospheric molecules across the outer solution boundary had to be changed to reflect the different geometry of the flux. (I.e., molecules were no longer coming across a curved outer boundary.)

4) The calculation of output quantities had to be modified to reflect the different positions at which the output was occurring.

3. SUMMARY OF WORK PERFORMED IN THE SECOND YEAR

Substantial work was accomplished in the past year in terms of added capabilities to the code as well as correcting "bugs". Sometimes the distinction between these two types of work is unclear, since a new feature

is frequently required to overcome an unanticipated (physically or numerically real) situation which causes the program to either fail or function poorly. Most of the "bugs" are in fact of this type with very few being due to simple programming or logic error. This is not surprising, since all new capabilities and routines are subjected to tests before they are installed in the code, so simple mistakes are usually discovered before they are part of the code. All of the pertinent work is described in the subsections below.

3.1 New Code Features

3.1.1 Surface Statistics

The purpose of a contamination code cannot be served unless the flux to, and buildup of, contaminants on the surface elements can be described. The ability to keep statistics for species fluxes on the various surface elements was added in the past year. The requests are input with the surface element definitions, and involve listing the species for which surface flux information is desired for the given surface element. The code automatically sets up the required storage location, advances a counter whenever a molecule of a selected species strikes the surface element, and generates output to show the derived species flux. As part of this calculation, it was necessary to calculate the areas of each surface element, so the derived flux can be given as a number of molecules per unit time per unit area.

3.1.2 Brook Core Model

Similarly, a contamination model cannot function without sources of contaminants. The code has been designed in a modular fashion, so that various sources of contaminants can be "plugged in" as desired. The Brook core model was selected as the initial source since it is a good description for the main exhaust flow from a rocket, and experience with it existed from the earlier plume codes. This model does not provide a good description of the mass flow at large angles from the thrust axis, and it is therefore inappropriate to describe the direct contamination from the engine exhaust to the shuttle. It is reasonable, however, in describing the portion of the exhaust which is blown onto the shuttle surfaces after suffering collisions with the ambient atmospheric molecules.

The core model makes use of the fact that the plume gases expand upon leaving the exit plane and adopt an essentially radial flow profile over a distance on the order of a few exit radii. Since this distance is small compared to the other length scales of interest, it is appropriate to

replace the nozzle by a point source of exhaust molecules traveling at their thermodynamic limiting speed (i.e., with zero translational temperature) with a number density distribution (before collisions with atmospheric species) given by

$$n_e = \frac{B}{r^2} f(\theta) \quad , \tag{1}$$

where B gives the axial number density decay and θ represents the angle from the thrust axis. The particular form for $f(\theta)$ is an asymptotic form of that proposed by Brook,[2] namely

$$f(\theta) = \exp\{-\lambda^2[1-\cos(\theta)]\} \quad , \tag{2}$$

where

$$\lambda^2 = \frac{1}{1-C_{fr}} \quad , \tag{3}$$

$$C_{fr} = \frac{1}{2}[1+\cos(\theta_n)]\left(\frac{u_o}{u_m}\right)\left[1+\frac{1}{\gamma M_o^2}\right] \quad , \tag{4}$$

$$\left(\frac{u_o}{u_m}\right) = \left[1+\frac{2}{(\gamma-1)M_o^2}\right]^{-.5} \tag{5}$$

and

$$B = \frac{1}{2\pi} n_o A_o \lambda^2 \left(\frac{u_o}{u_m}\right) \quad . \tag{6}$$

In the above relations, u_o, M_o, n_o and A_o denote the exit velocity, Mach number, number density and area, respectively, θ_n is the nozzle divergence half angle and u_m and γ are the thermodynamic limiting speed and the exhaust ratio of specific heats.

3.1.3 Interface of Shuttle Model with Calculational Grid

The melding of the three dimensional Cartesian cell grid structure with the arbitrary geometry of the space shuttle orbiter (or, generally, any spacecraft) posed a problem. The difficulty arose from the fact that the cell structure is not molded around the orbiter, so the boundaries of the orbiter do not correspond to cell boundaries.

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2. Brook, J. W., "Far Field Approximation for a Nozzle Exhausting into a Vacuum", Journal of Spacecraft and Rockets, 6(5), May 1969, pp. 626-628.

The cells are used for two purposes in the simulation: 1) to provide positions for flow field output quantities and 2) to define the location of possible collision partners for molecules. For either purpose, but especially for the second one, it is desirable that macroscopic properties do not change appreciably across the cell. This is because the only spatial requirement on two molecules to qualify as collision partners is that they lie within the same cell; if the cell is uniform, then it is argued that a sample molecule could equally well be found anywhere within the cell, and its precise location in the cell is ignored in the collision sampling process. (This assumption is not made arbitrarily, of course; it results in a substantial computational simplification. See Ref. 3 for details.)

There is a problem with this assumption when pieces of the shuttle penetrate into a cell. The general collision sampling procedure would allow, for instance, a molecule above a wing to collide with a molecule below a wing. It is an inherent contradiction to assume that the contents of a given cell are uniform and that a piece of the shuttle penetrates the cell since the shuttle piece defines a length scale on the order of cell dimensions.

The resolution that was achieved was to analyze the cell and shuttle geometries to tag those cells which contained pieces of the shuttle, and to disallow collisions in those cells. As the cells become smaller, the neglected collisions become insignificant, so this is formally a source of error associated with finite grid size (an inherent part of any such calculation). It was judged better to not allow the very small number of legitimate collisions in these cells than to allow momentum transfer between molecules separated by a solid surface. It is important to emphasize that this approximation only has to do with molecular collisions. Direct contamination from a source to a surface still occurs, since it has nothing to do with the cell structure at all.

3.1.4 Spherical Coordinate Transformation Near Sources

There was another feature added to the code to address a problem similar to that discussed above. This problem results from the fact that for a concentrated source of contaminants such as the Brook core, the cell dimensions of cells adjacent to the source are of necessity comparable to

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3. Elgin, J. B., "Getting the Good Bounce: Techniques for efficient Monte Carlo Analysis of Complex Reacting Flows", Report SSI-TR-28, Spectral Sciences, Inc., Burlington MA, 1983.

the distance from the source. Hence, it is impossible for conditions within the cell to be considered uniform. (I.e., for instance, the density of molecules from a point source goes from infinity at the point source to some finite number at the other end of the cell containing the source.) Since conditions within the cell cannot be uniform, the assumption that position within the cell does not matter when selecting collision partners cannot be justified. Consider, for instance, two molecules leaving the source: one traveling mainly upward and one traveling mainly downward. These two molecules have a substantial relative velocity between them, and therefore would be likely candidates to be selected for collision. However, since they started at the same point heading in opposite directions, they should not physically be able to collide.

A simple resolution to this problem is to express the exhaust velocity elements in spherical polar coordinates, centered at the source. In these coordinates, every molecule leaves the point source with the same velocity in the direction of the spherical radius vector. Expressed in spherical polar coordinates, the relative velocity between the two molecules mentioned above disappears. Whenever the density in a cell is large compared to the ambient density, SOCRATES searches for the nearest point source and transforms the velocity components to a spherical coordinate representation with respect to that source. Collisions are carried out in the transformed coordinates, and then they are transformed back to Cartesian coordinates after the collision sampling. This completely eliminates the problem.

3.1.5 Cells with Enhanced Density

For a concentrated source of molecules, such as the Brook core source described above, a problem can arise with statistics. The problem relates to the expanding nature of the source molecule cloud as it travels away from the source. That is, consider the molecules emitted from the source in the time interval Δt. Initially, these molecules will be concentrated in one or two cells surrounding the source. As time increases, these same molecules will spread out and encompass more and more cells. Hence, the natural spreading of the source molecules produces fewer and fewer real molecules per cell as cells get further away from the source.

This physical tendency contrasts with the numerical desirability of keeping the number of simulated molecules per cell as an approximate constant - enough to get meaningful collision statistics but few enough to keep from overflowing code dimensions. To accommodate the physical reality to the numerical requirement, the code uses dynamically adjusted statistical weighting factors. As molecules cross cell boundaries, they are replicated and their statistical weighting factors are corresponding

reduced. The number of simulated molecules is increased, but their statistical weight decreases correspondingly to keep the number of physical molecules the same. The procedure by which molecules are replicated when they cross cell boundaries is referred to as "cloning" (see Ref. 3), and it is a procedure which has some drawbacks. Accurate statistics are better obtained by having many different molecules rather than having many copies of just a few molecules.

To lessen the statistical drawback of cloning, some cells are allowed to have significantly more distinct molecules than others. Since a simulation typically is run with thousands of cells, the increased molecule quota for a few cells has no significant impact on the overall storage requirement for the code. The particular cells that are chosen are ones which contain or are adjacent to a concentrated source. This feature in the code compensates for the natural spreading of molecules as they leave the source and produces less cloning and, therefore, better statistics. The feature has been implemented in the SOCRATES code.

3.2 Identified and Rectified Bugs

3.2.1 Penetrating Molecules

During the testing of the routines for intersecting a molecule with the shuttle surfaces, a problem was uncovered which resulted from a combination of numerical roundoff error and "bad luck". (It is axiomatic that anything that can go wrong in a Monte Carlo code eventually will go wrong; improbable events simply take longer to show up.)

Surface intersections were computed for each molecule, and the time for the intersection was stored together with other information in the molecule's state vector. This procedure meant that as a molecule progressed along a straight line trajectory, its intersection did not have to be continually recomputed; the recomputation was required only when the trajectory changed due to a collision. (See Section 2.)

The problem was that as a molecule was advanced along its trajectory in many small time steps, accumulated numerical error slightly changed the time at which an intersection would occur. Normally, this made no difference to the solution. However, if the error became enough to change the time step in which the intersection occurs, then an intersection could be "missed", and the molecule would go through a solid surface. Although such an occurrence would probably be statistically insignificant, the feeling was that impossible events should be discouraged as much as possible.

The bug was eliminated through a combination of two changes. Firstly, logic for "backing up" a molecule when an intersection was missed was instituted. When a scheduled intersection isn't found, a molecule is backed up 0.1% of the time step along its trajectory and the intersection is searched for again. This procedure by itself was sufficient to rectify the problem wherever it has occurred to date. A second change was implemented, however, to make the occurrence of the problem much less frequent. The change involved shifting the time reference from the time at the start of the simulation to the time at the start of each step. Each step is then carried out for a time period between 0 and Δt_m, the solution time step. (After the time step, Δt_m is subtracted from the time at which the intersections are to occur for all the molecules, as well as from the collision time counters.) This seemingly minor change means that the full precision of the computer is available for the time variable whereas previously it was diminished as the simulation progressed. (I.e., after a thousand steps, an overall time counter loses three significant digits when comparing times on the order of the time step.)

3.2.2 Back-To-Back Surface Problem

A shuttle surface such as a wing was considered to have negligible thickness in the first shuttle model, so it was modeled as back-to-back planar segments; one for each of the two outward normal directions. (The use of the outward normal as a critical piece of surface information allows molecule-surface interactions to be calculated efficiently, since the molecule's velocity vector and a planar surface's outward normal must have a negative dot product for an intersection to be possible. This allows roughly half of the surfaces to be immediately eliminated when searching for intersections.) Due to the neglect of surface thickness, when a molecule intersected with such a back-to-back surface, it bounced back and forth between the two surfaces indefinitely without ever moving. Once recognized, this was a simple oversight to correct.

3.2.3 Issues Relating to Uncollided Source Molecules

A molecule which leaves a point source is referred to as a virgin source molecule until it suffers its first collision. Two such molecules cannot collide, since they originate at the same point and travel in different directions. For cells adjacent to the source, the unphysical collisions are prevented via the spherical transformation discussed in Section 3.1.4, but when cell densities become lower this transformation becomes computationally cumbersome and is not used. However, it is still true that the first collision suffered by a virgin source molecule cannot be with another virgin molecule from the same source. These unphysical

collisions are prevented everywhere in the solution by putting a tag on these molecules and checking the tags during collision sampling. The tag is removed, of course, once a molecule undergoes its first collision.

Several issues arose and were solved with regard to virgin source molecules during the past year. The previous implementation did not recognize that virginity should be preserved when a molecule undergoes a spontaneous radiative decay to change from a vibrationally excited species to a ground state species. Since there is no momentum change in this process (ignoring, of course, the photon momentum), the molecule still qualifies as a virgin, even though it is no longer the same species that was emitted from the source. (Distinct vibrational states are treated as separate species in the simulation.)

During the collision sampling, if two virgin source molecules are initially selected as potential collision partners, they are immediately rejected and another pair is tried. This process has the capacity to bring the collision sampling to a screeching halt if the cell is populated solely by virgin source molecules; the program could search forever but it would never find an acceptable collision pair. A similar problem arises when molecular clones are in the same cell; since they have precisely the same velocity vector, the relative velocity between them is zero and they can never be selected for collision. (See Ref. 3) Special logic had to be implemented that recognized these situations when they occurred and temporarily bypassed the collision sampling for the cell in question.

Lastly, consider the situation when a single outside molecule enters a stream which is overwhelmingly dominated by a nearby source. When it collides with a virgin source molecule, the virgin tag is removed and both molecules can then collide with the virgin source molecules. There can follow an avalanche of collisions, which removes the virgin tag from many molecules. However, even though there are many collisions, the introduction of the single foreign molecule cannot have a significant impact on the overall momentum of the stream. The result of these many collisions is to have all the molecules once again traveling with essentially the virgin source velocity vector. When this is true, the relative velocity between the molecules becomes less and less, and it becomes harder and harder to find an acceptable pair of molecules for a collision. The fix that was put in to avoid this problem was to allow, at least for Monte Carlo fluid mechanics, the regaining of virginity. When the velocity becomes within a small tolerance of the virgin source conditions, the virgin tag is restored.

4. SAMPLE CALCULATION

4.1 Case Description

In order to check out the code and demonstrate some of its current capabilities, a sample calculation was undertaken. The calculation was for a case with the simplified shuttle model flying at an altitude of 200 kilometers at a velocity of 7 km/s. The shuttle was taken to be flying at a normal aircraft orientation (i.e., nose into the oncoming stream) and firing an RCS thruster upward from its nose. The geometry of the calculation, with the coordinate system, is depicted in Figure 2.

The calculation was performed for a steadily firing engine of 860 pounds thrust, with an exhaust composition as shown in Table 1.

Table 1. Exhaust Composition for Sample Calculation.

Species	Mol. Weight	Mole Fraction
H_2	2.00	0.1800
H_2O	18.00	0.3284
CO_2	44.00	0.0472
Other	27.35	0.4444

The composition shown in Table 1. was chosen to show the specific effect on exhaust species molecular weight on the development of the contamination cloud. Hence, light (H_2), medium (H_2O) and heavy (CO_2) molecules were explicitly carried in the simulation, and all other species were grouped together into a species called "Other", with a molecular weight given by the mean of all the remaining exhaust species.

4.2 Contamination Cloud Results

The presentation of quantities as a function of three spatial dimensions is always somewhat difficult. The approach that has been taken is to show isodensity contours for planes perpendicular to the direction of the oncoming wind. That is, referring to Fig. 2, constant values of X were chosen and isodensity contours of the three species are shown as a function of Y and Z. X locations of 0, 500, 1000 and 1500 meters were chosen, showing the spread of the contamination cloud upstream. (It is perhaps surprising that anything penetrates upstream into a 7 km/s wind, but the atmospheric mean free path for this calculation is approximately 325 m, so

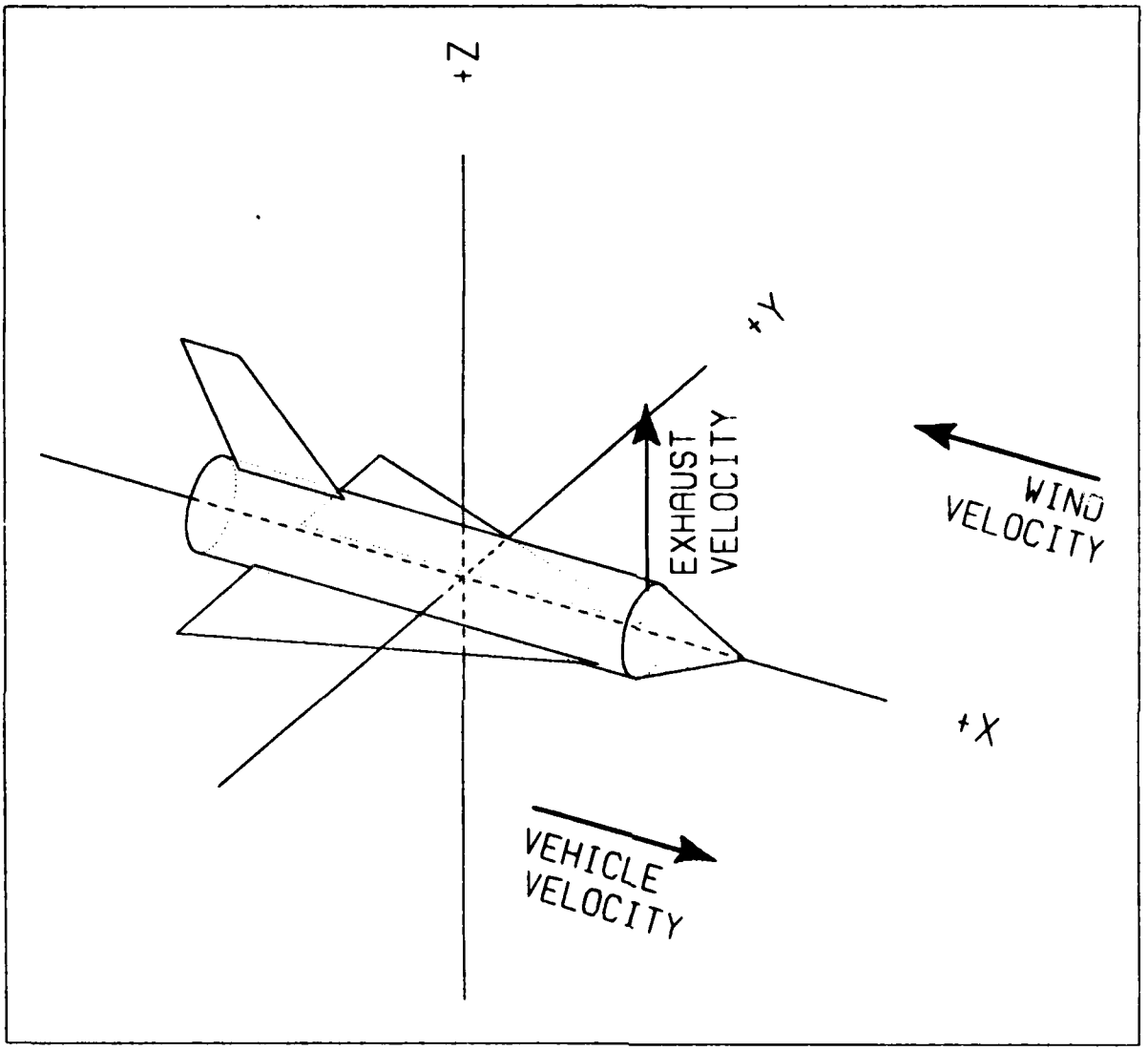

Figure 2. A Schematic of the Sample Shuttle Problem Showing the Coordinate System and Orientation of the Calculation.

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the effects of normal molecular diffusion are greatly exaggerated beyond their usual length scales.) The results for H_2 are shown in Figs. 3-6, for H_2O in Figs. 7-10 and for CO_2 in Figs. 11-14. These figures quantitatively

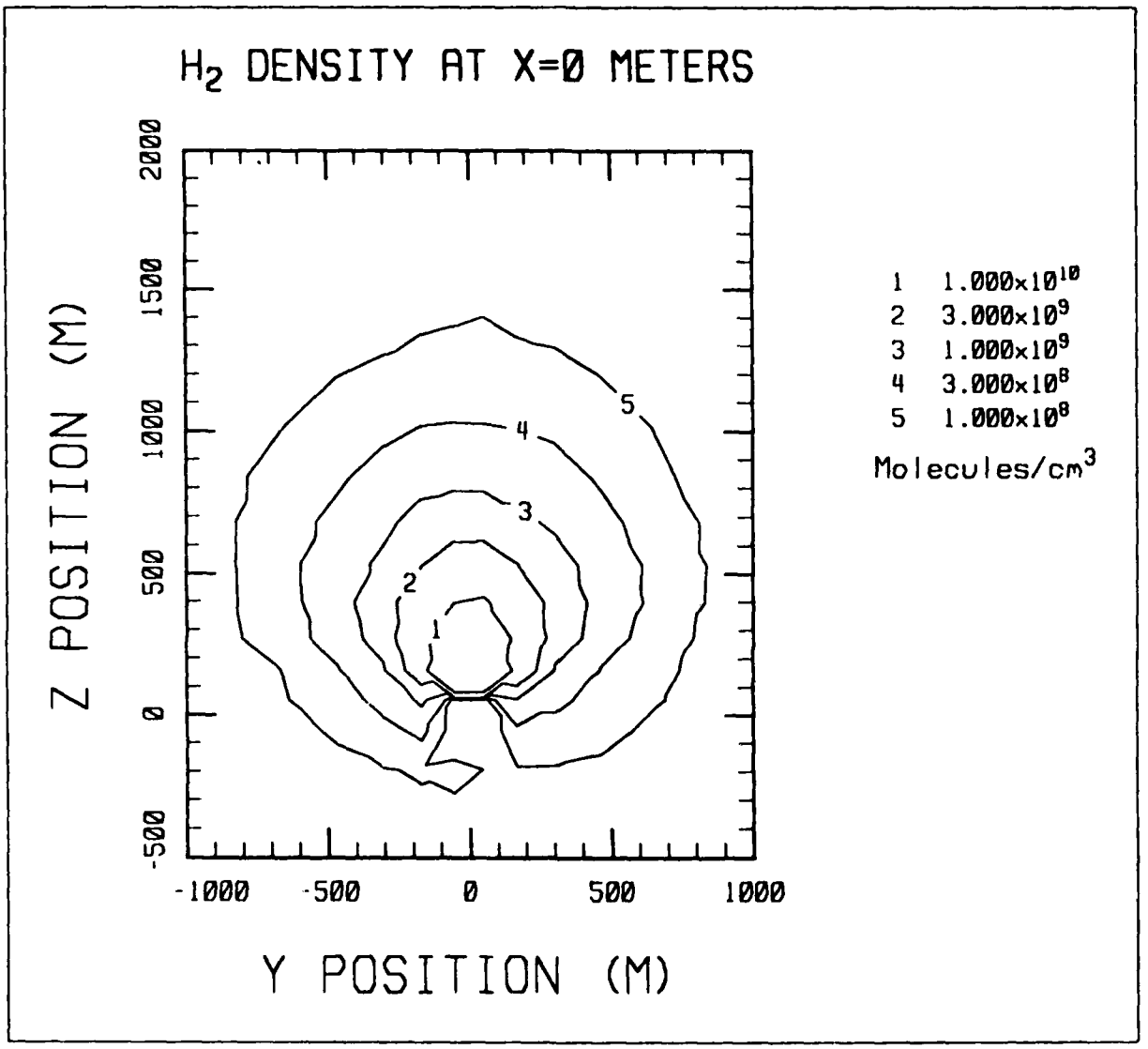

Figure 3. A Contour Plot of the H_2 Number Density at an X Location of 0 Meters.

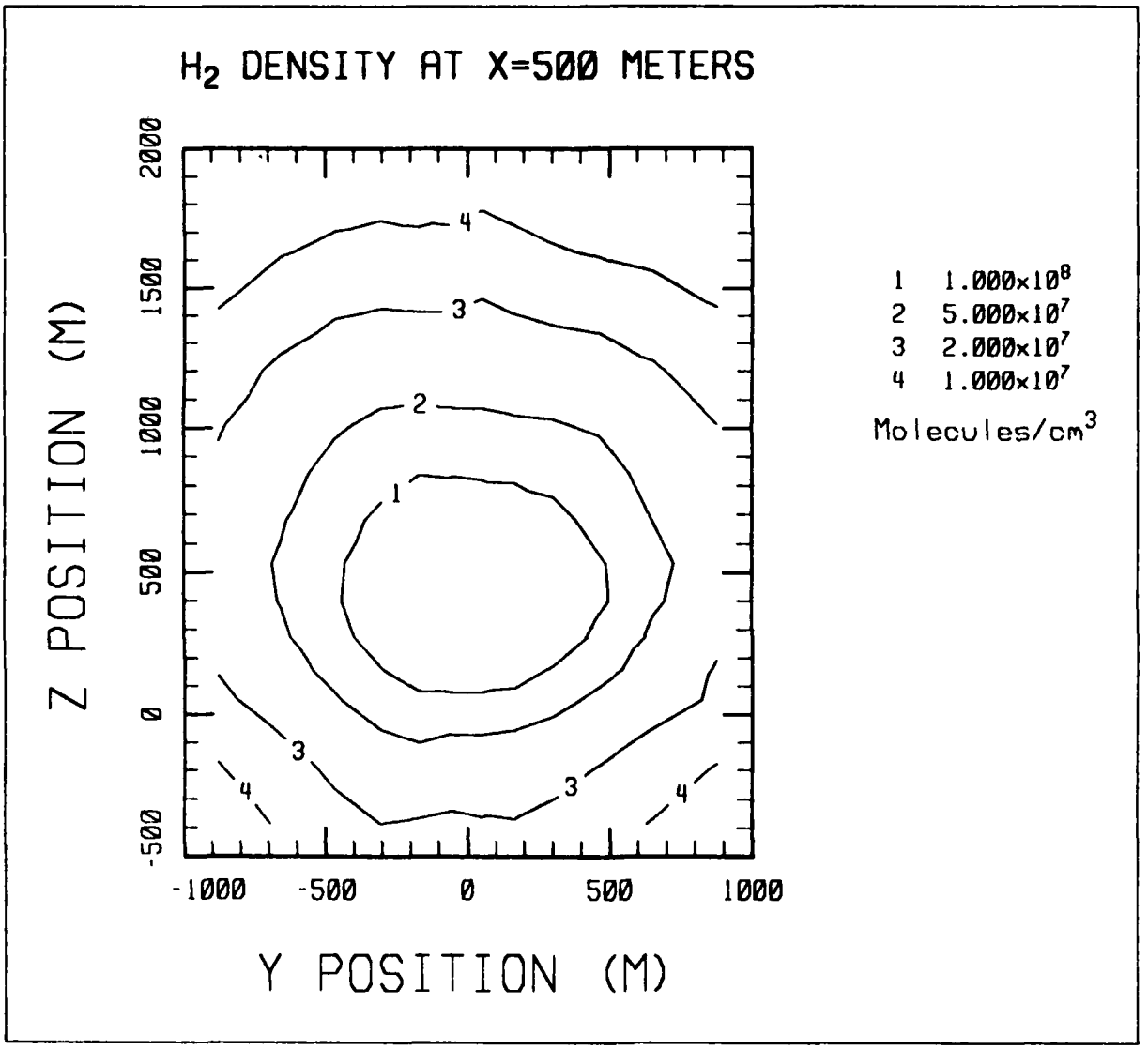

Figure 4. A Contour Plot of the H_2 Number Density at an X Location of 500 Meters.

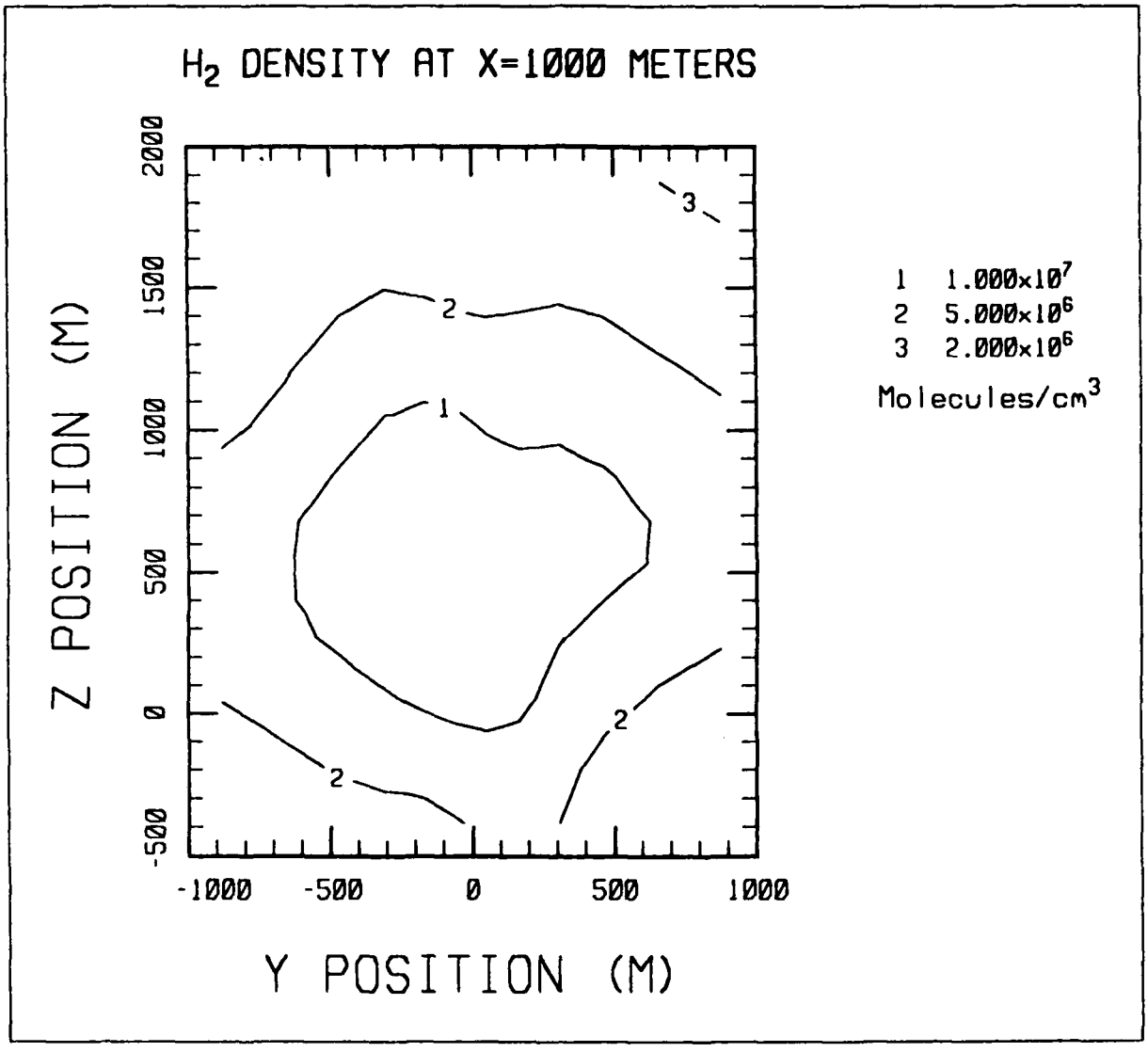

Figure 5. A Contour Plot of the H_2 Number Density at an X Location of 1000 Meters.

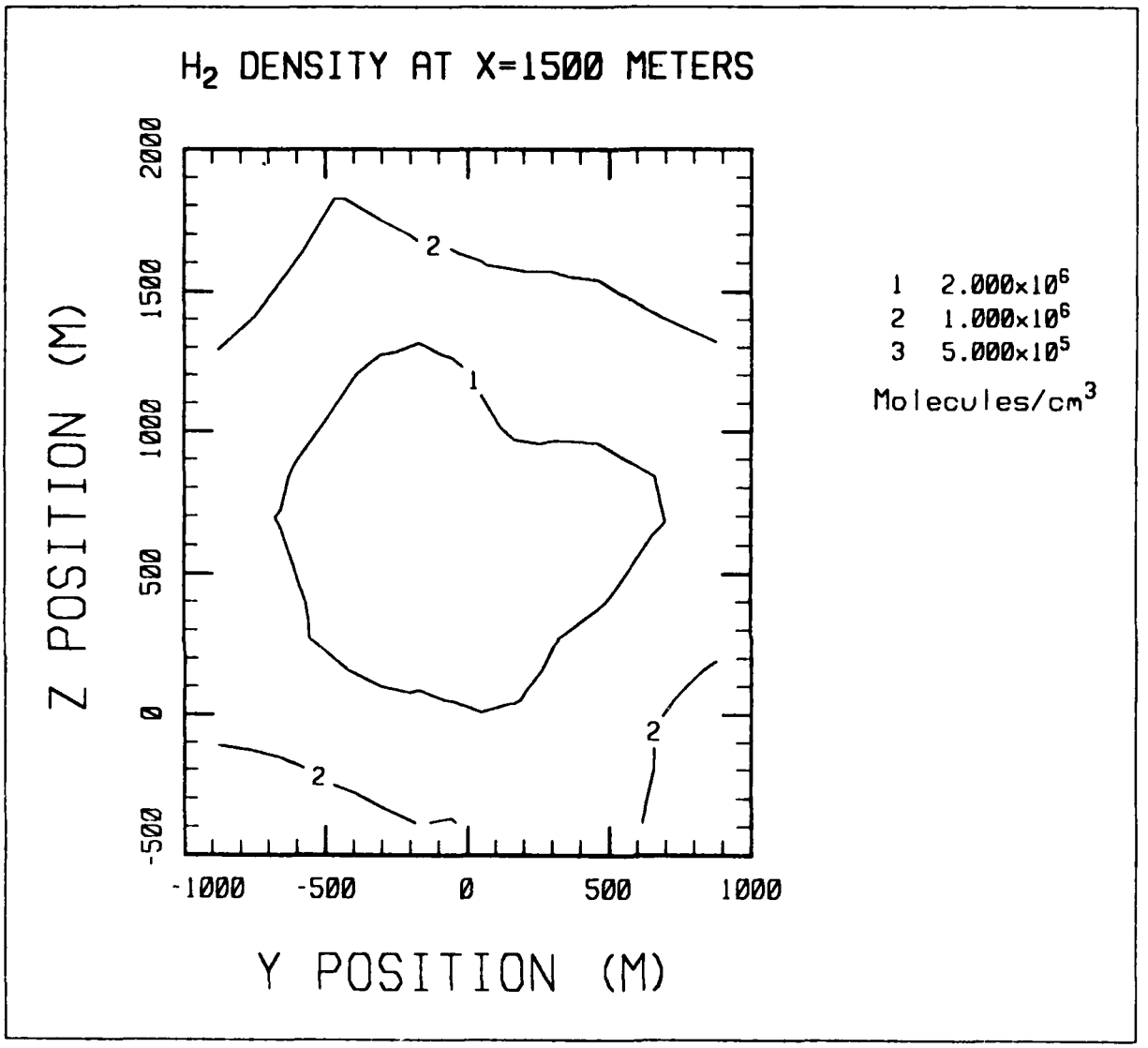

Figure 6. A Contour Plot of the H_2 Number Density at an X Location of 1500 Meters.

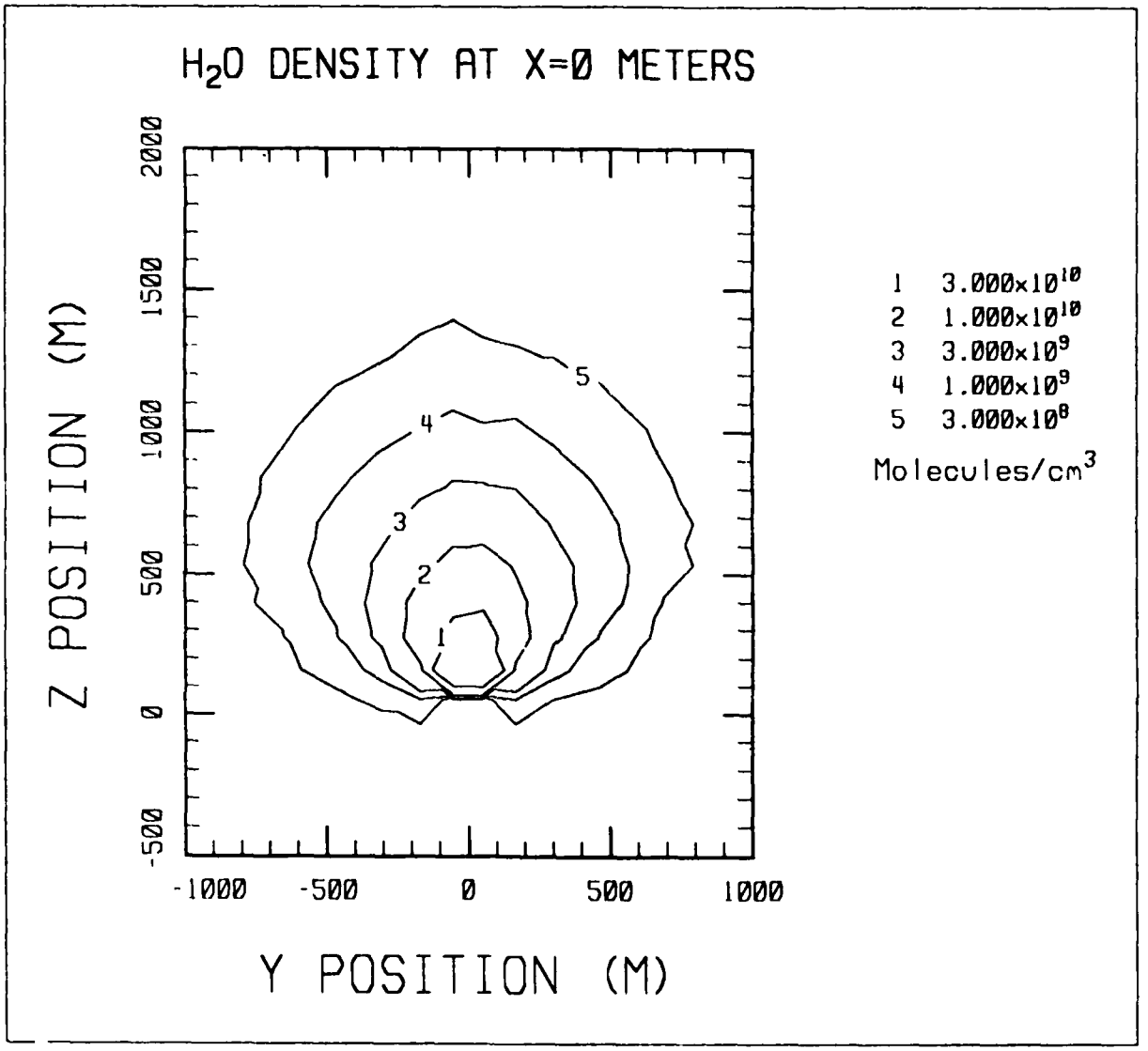

Figure 7. A Contour Plot of the H_2O Number Density at an X Location of 0 Meters.

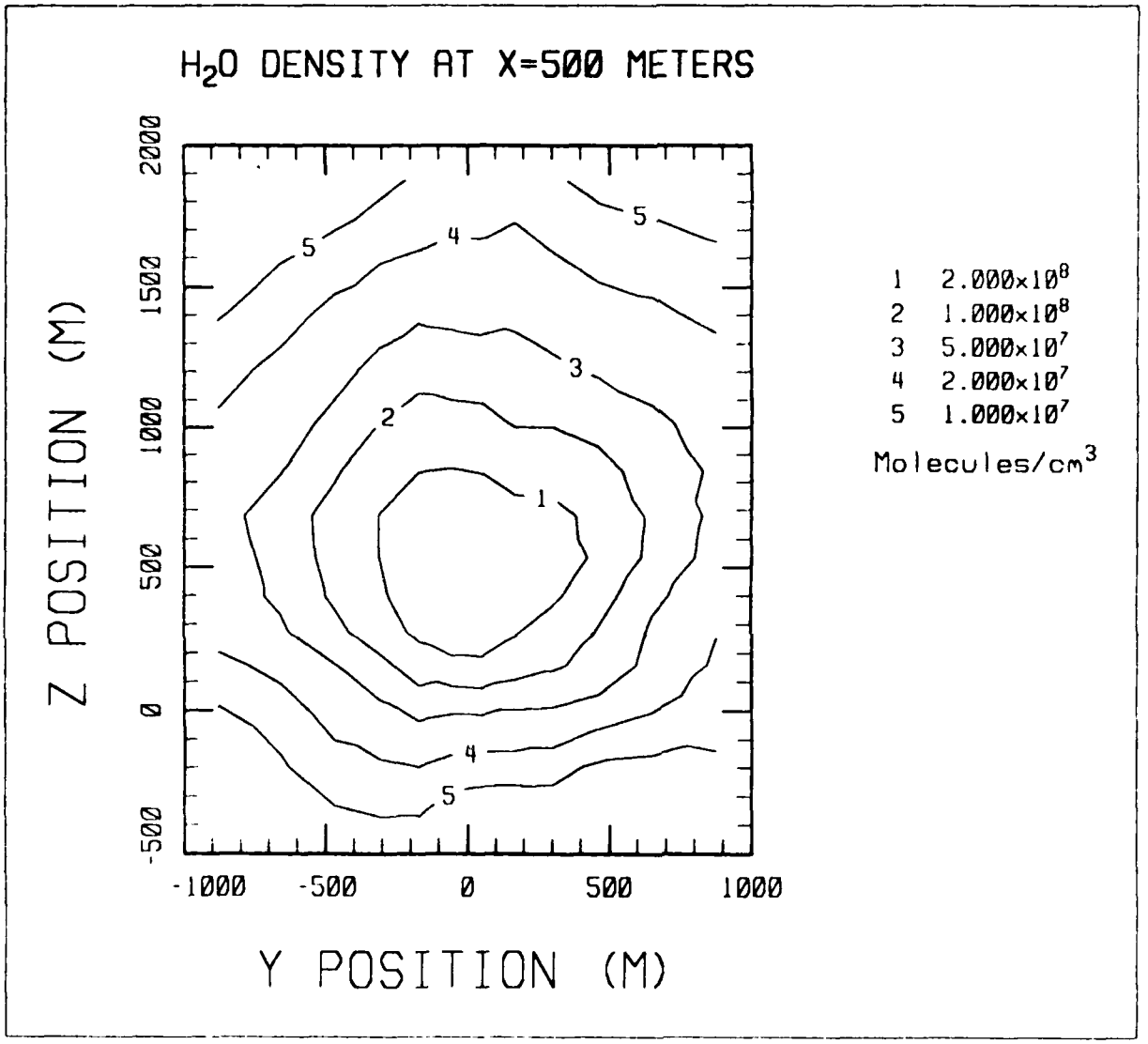

Figure 8. A Contour Plot of the H_2O Number Density at an X Location of 500 Meters.

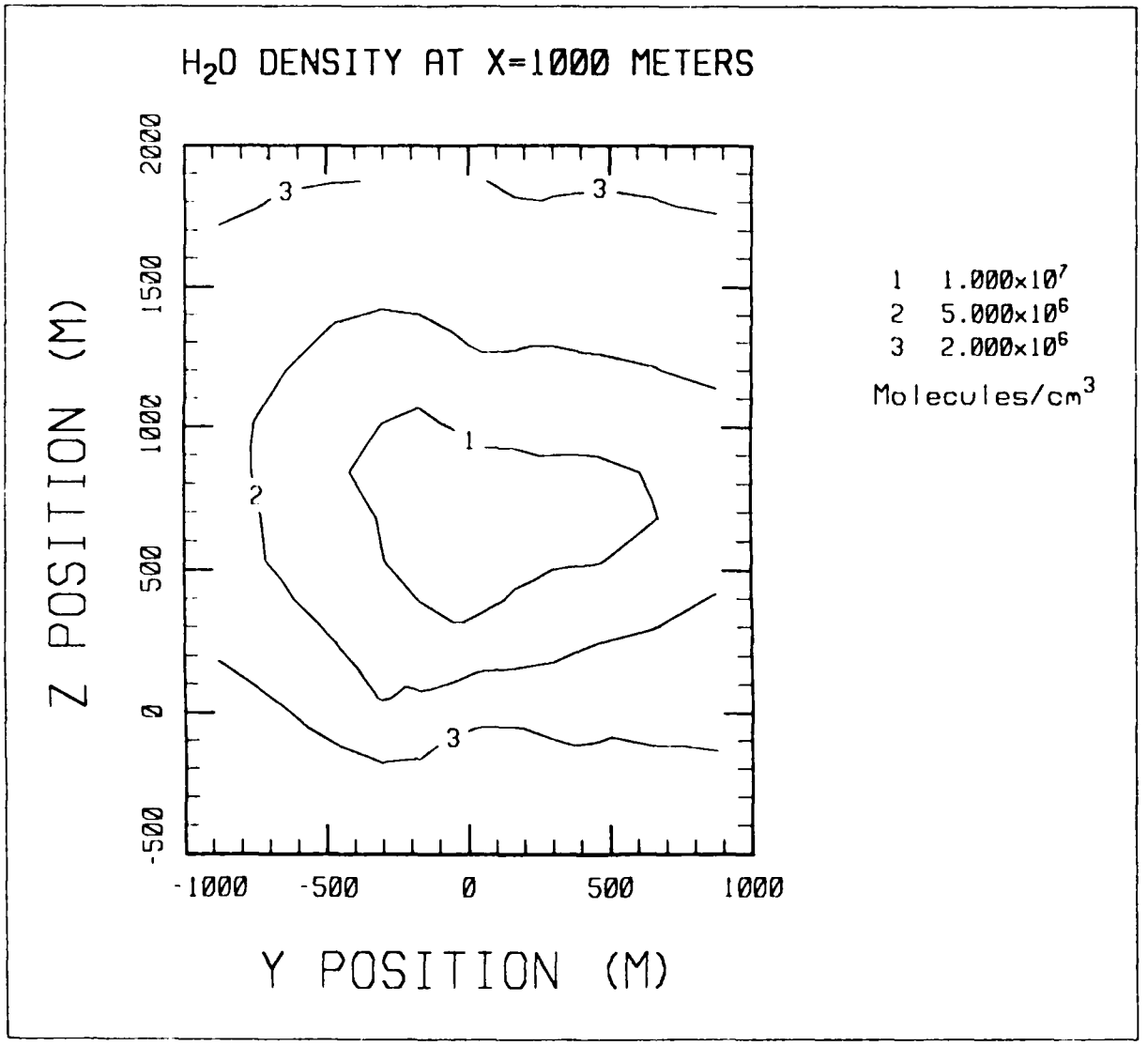

Figure 9. A Contour Plot of the H_2O Number Density at an X Location of 1000 Meters.

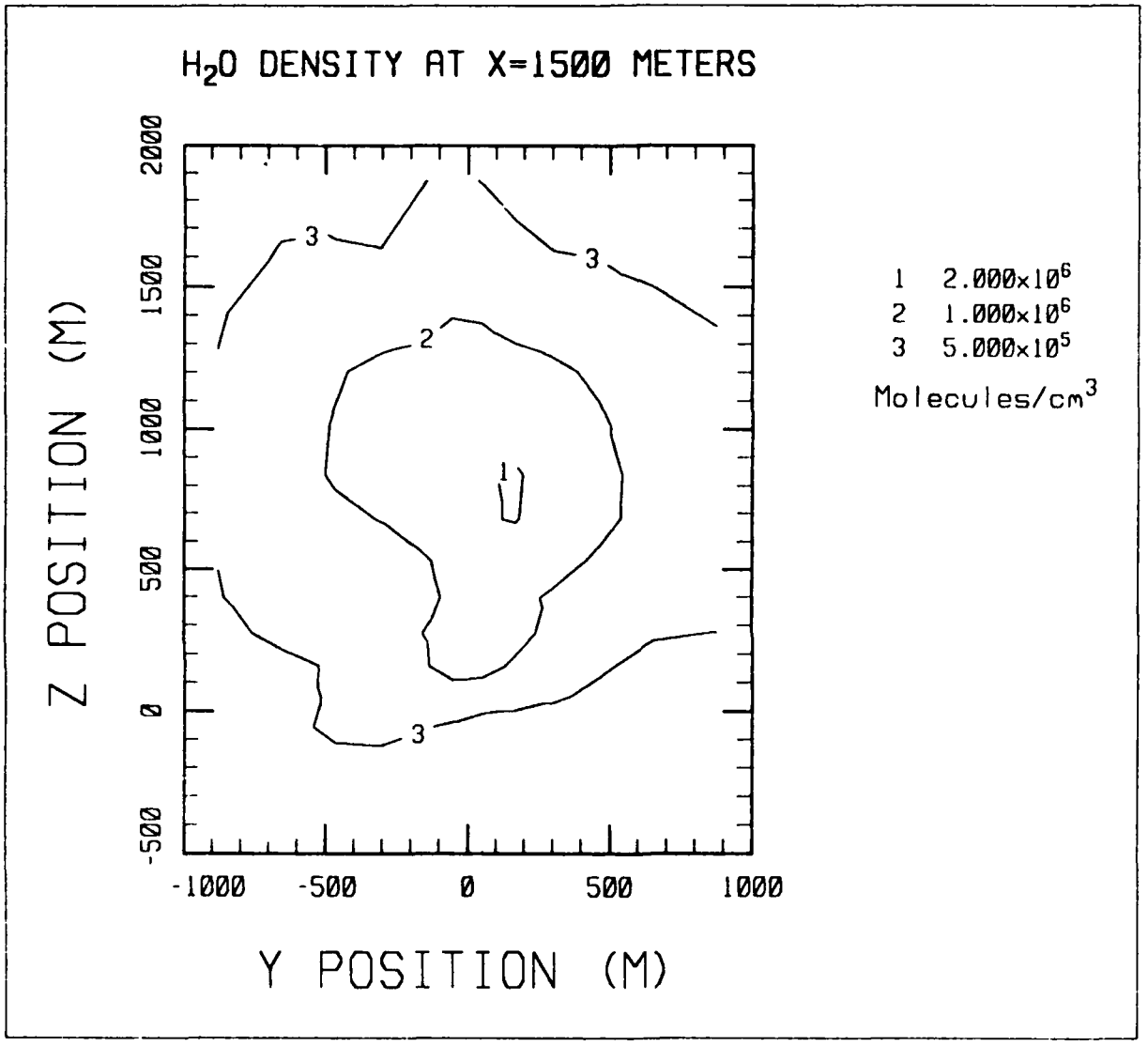

Figure 10. A Contour Plot of the H_2O Number Density at an X Location of 1500 Meters.

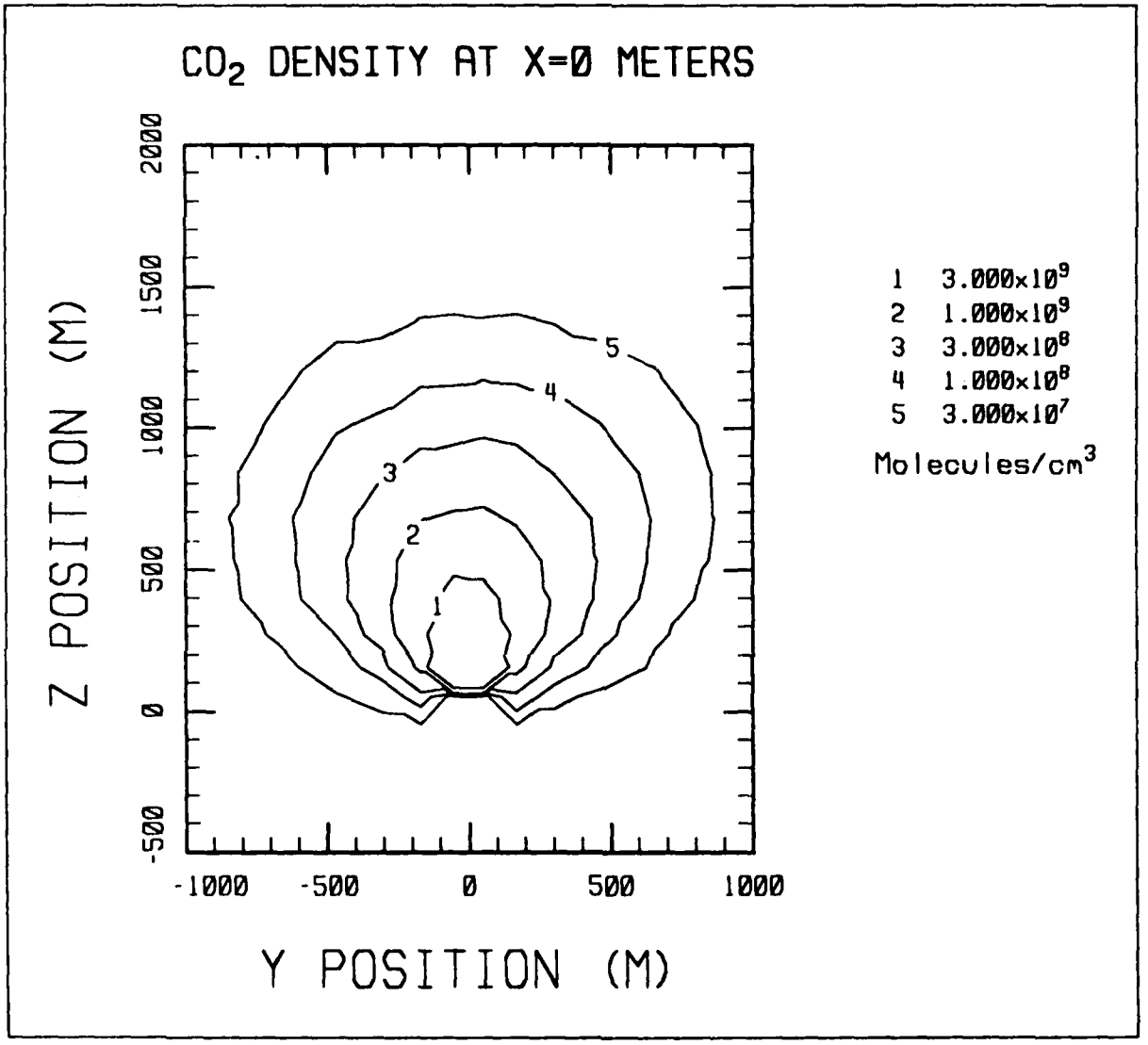

Figure 11. A Contour Plot of the CO_2 Number Density at an X Location of 0 Meters.

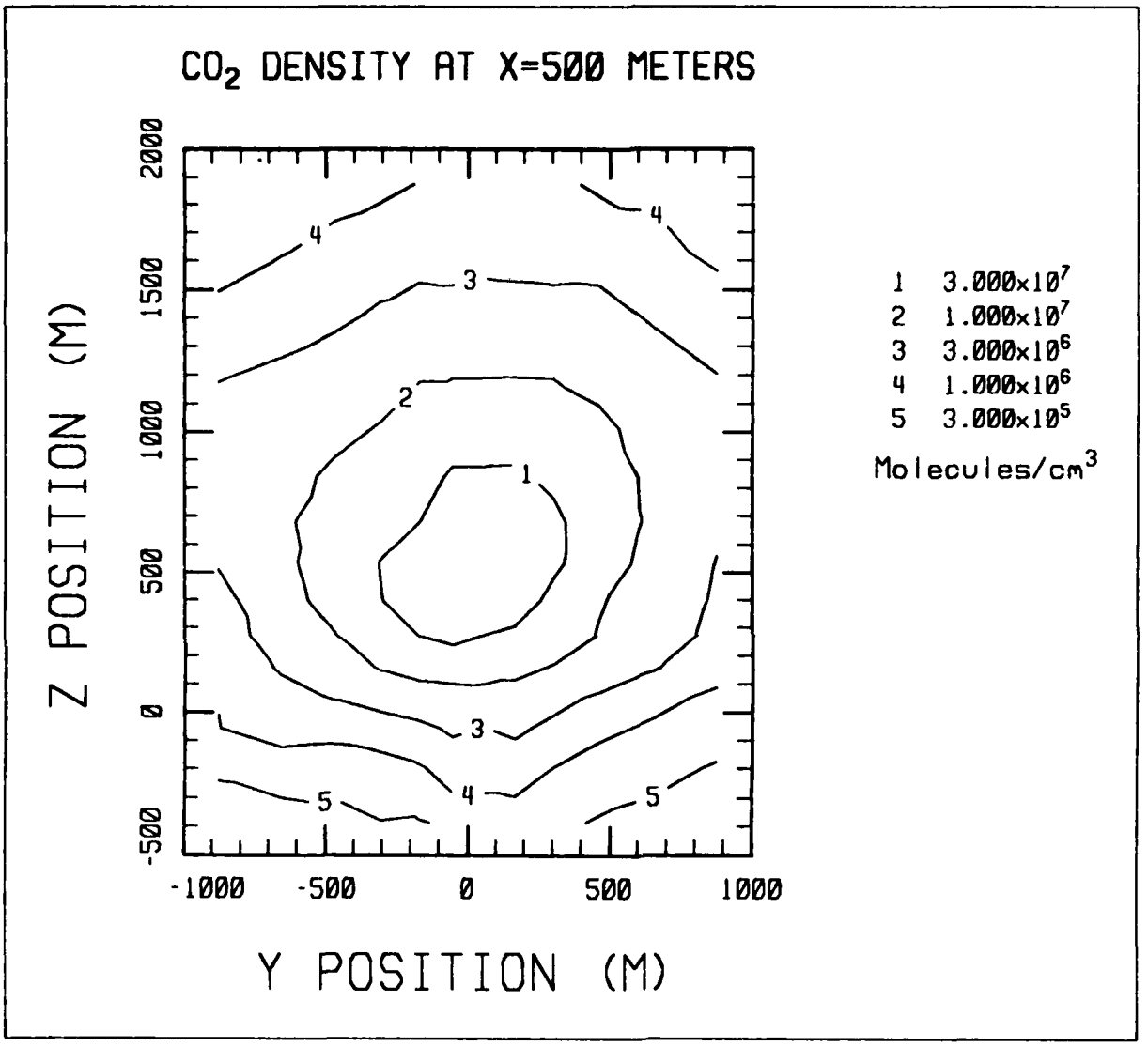

Figure 12. A Contour Plot of the CO_2 Number Density at an X Location of 500 Meters.

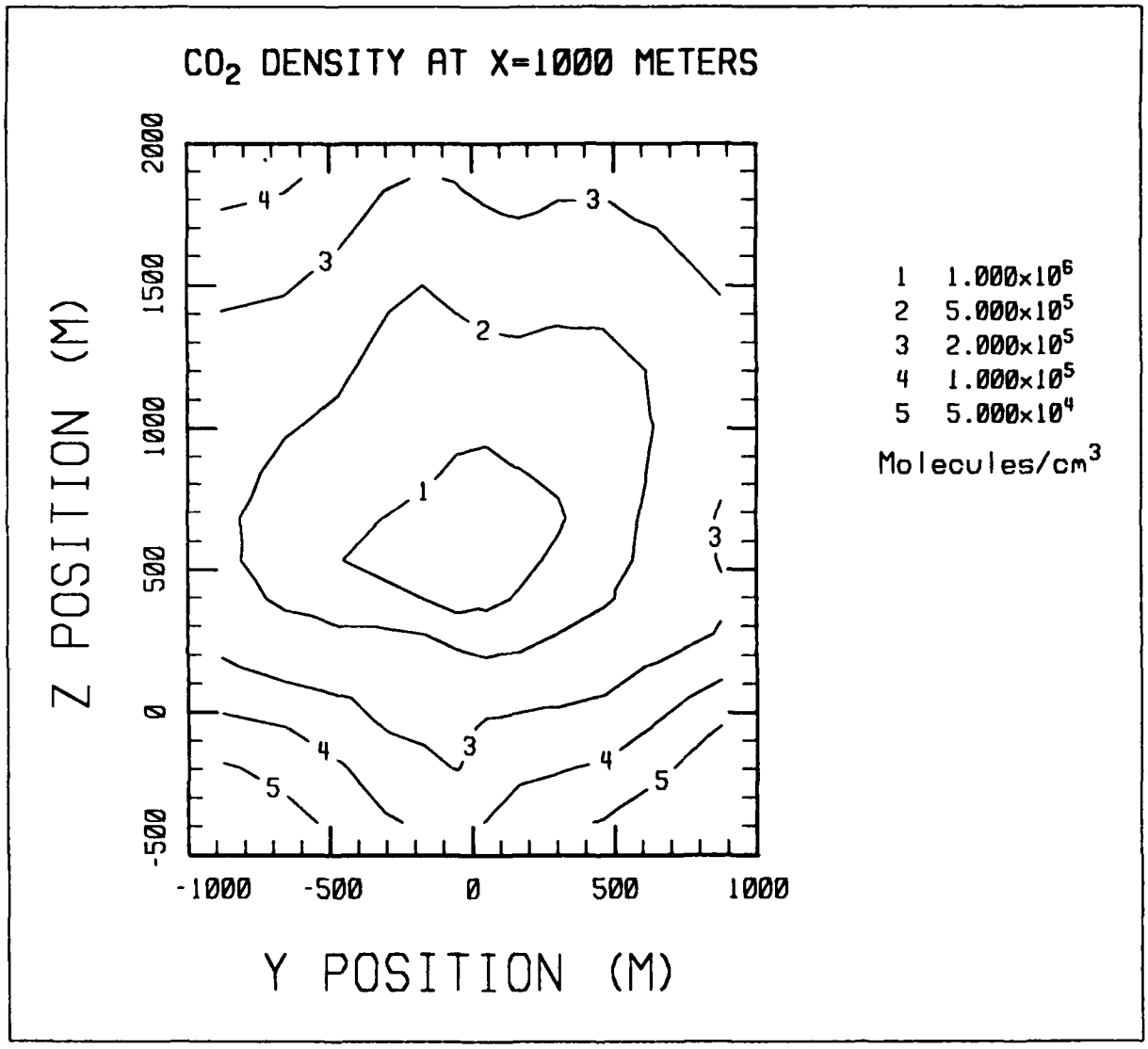

Figure 13. A Contour Plot of the CO_2 Number Density at an X Location of 1000 Meters.

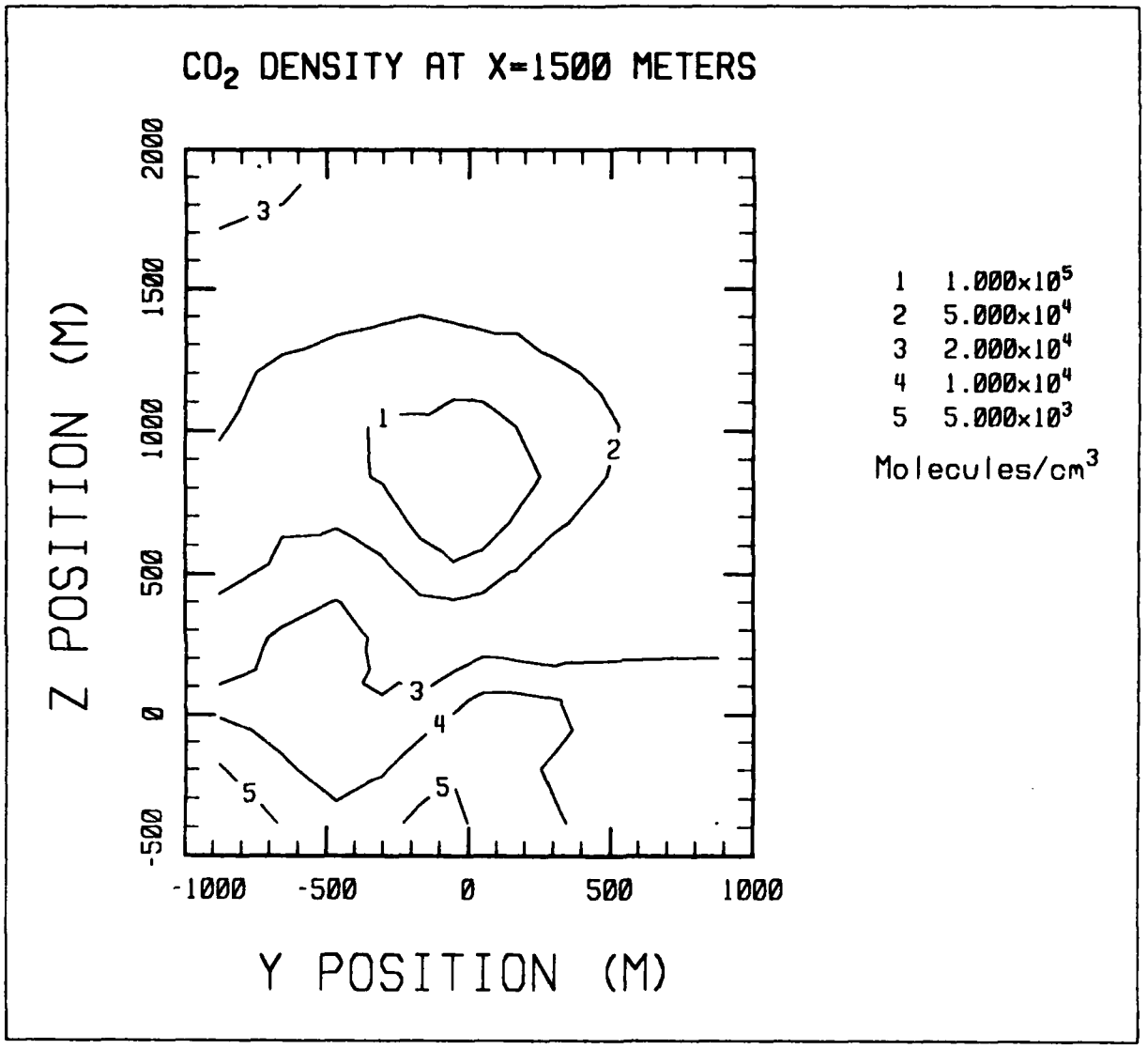

Figure 14. A Contour Plot of the CO_2 Number Density at an X Location of 1500 Meters.

demonstrate what could have been predicted qualitatively, namely, that H_2 is more effective at traveling upstream than the other two molecules. This is partially because H_2 has a smaller cross section (and therefore a greater mean free path) than the other molecules, but mainly because its smaller molecular weight results in greater molecular velocities. It makes the most of the time it has between collisions. This point is made more directly in Fig. 15, where the number densities of the three species are shown at a location of 1 km above the shuttle, as a function of the upstream coordinate. Within the statistical scatter, there is no apparent difference in the upstream decay rate for H_2O and CO_2, but relative to these molecules H_2 gains approximately an order of magnitude in density at an upstream distance of 2 kilometers. (At this distance it is probably comparable to the atmospheric concentration of H_2, although no atmospheric H_2 was included in the calculation. The point that is being made, however, is simply that light molecules are better at making it upstream and then being blown back into the shuttle area.)

4.3 Surface Contamination

Expected surface contamination results were not obtained for this run. The reason is that the altitude was high enough that the atmospheric mean free path was greater than shuttle dimensions, and the solution region had to extend to many mean free paths to describe the contaminant cloud. The resultant large cell size meant that molecular interactions with the shuttle became sufficiently improbable that none occurred. This outcome will be avoided in future runs by two approaches.

Firstly, for lower altitudes and/or contaminant sources with smaller characteristic length scales, the grid will be substantially tightened. This will enable the shuttle to occupy many cells rather than a small portion of a cell. The result will be the intended statistics.

Secondly, for future runs of similar length scales to that presented here, use will be made of the natural separation of length scales which led to the problem. (I.e., the shuttle being small compared to the characteristic plume length and the atmospheric mean free path.) In these cases, the shuttle itself has a negligible effect on the contamination cloud. Judicious techniques can turn this problem into an advantage. Hence, if the code makes a distinction between scattered and unscattered exhaust molecules, then direct surface contamination is easily calculated from impingement of unscattered exhaust molecules onto shuttle surfaces. The scattered cloud, having a much larger length scale than the shuttle, can have its velocity and temperature (more precisely, its velocity distribution spread) calculated in the vicinity of the shuttle. These quantities then can be used to calculate contamination on any surface directly.

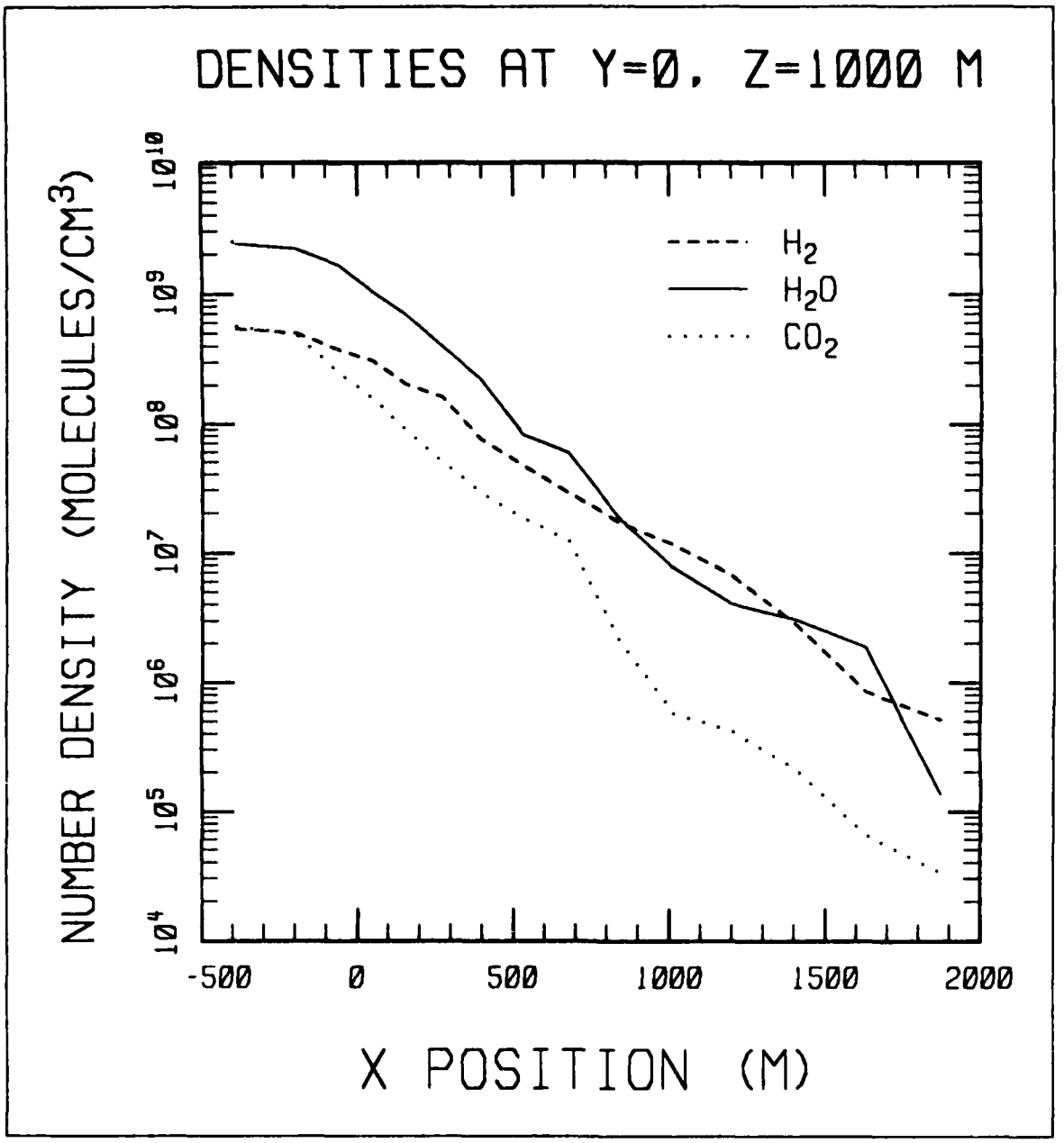

Figure 15. A Comparison of the Upstream Density Decay for the Three Molecules Carried in the Sample Calculation.

5. REMAINING WORK ON CONTRACT

Initial development of the SOCRATES is continuing, and its status will be improved before the end of the current contract. It is expected that the Simons[4] model will be used to describe direct exhaust contamination of spacecraft surfaces. It will probably be necessary to use different statistical weighting factors for the boundary layer portion of the flow, since it is a small fraction of the total exhaust flow.

The surface interaction options will be expanded to allow for molecules adhering to surfaces, and statistics will be kept on the concentration of various contaminants on critical surfaces. The evaporator vents will also be described as a contaminant source as will, possibly, cabin leakage. Hence, at the contract end the SOCRATES code is expected to be a powerful tool for describing neutral contamination resulting from various sources, with the ability to describe complex gas phase chemistry and atmospheric interactions. The code will be documented with a user's manual and delivered to AFGL.

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2. Brook, J. W., "Far Field Approximation for a Nozzle Exhausting into a Vacuum", Journal of Spacecraft and Rockets, 6(5), May 1969, pp. 626-628.

3. Elgin, J. B., "Getting the Good Bounce: Techniques for efficient Monte Carlo Analysis of Complex Reacting Flows", Report SSI-TR-28, Spectral Sciences, Inc., Burlington MA, 1983.

4. Simons, G. A., "Effect of Nozzle Boundary Layers on Rocket Exhaust Plumes", AIAA Journal, 10(11), November 1972, pp. 1534-1535.

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